MIDTERM 1

ECE 371 – Fall 2019

MATERIALS AND DEVICES

UNIVERSITY OF NEW MEXICO

Tuesday September 24th, 2019

Time Limit: 1 hour 15 minutes

Exam is closed book and notes

Calculators okay

Some constants and equations are given on the last page

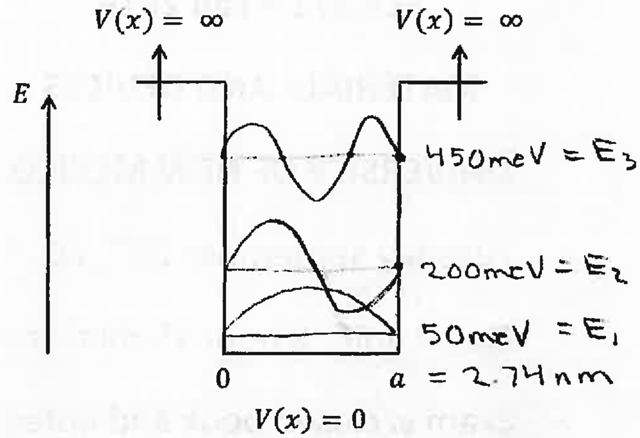
(100 points, 20% of course grade)

Name: Solutions

Score:____________

(20 points)

1. Consider an *electron* confined within an infinite potential well of width a as shown in the following figure. The potential is infinity outside of the well and zero within the well $(0 < x < a)$.



The wave functions are given by $\psi(x) = A\,sin\left(\frac{n\pi}{a}x\right)$ and the quantized energy levels are given by $E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$, where $A = \sqrt{\frac{2}{a}}$

a. (5 points) Design the well thickness (a) such that the first quantized energy level (E_1) is 50 meV above the bottom of the well.

b. (5 points) Using the thickness you obtained in part (a), determine the de Broglie wavelength of an electron in the second quantized energy level (E_2)?

c. (5 points) What is the probability of finding an electron in the first energy level (E_1) between 0 and $a/4$?

d. (5 points) Sketch the first three energy levels and their associated wave functions to scale on the well image above.

a. $E_1 = 50\,meV = 0.05\,eV \cdot \frac{1.6\times10^{-19}\,J}{eV} = 8\times10^{-21}\,J$

$E_1 = \frac{\hbar^2\pi^2}{2ma^2} \implies a = \sqrt{\frac{\hbar^2\pi^2}{2mE_1}}$

$a = \left[\frac{(1.054\times10^{-34}\,J\cdot s)^2\,\pi^2}{2(9.11\times10^{-31}\,kg)(8\times10^{-21}\,J)}\right]^{1/2} = 2.74\times10^{-9}\,m = \boxed{2.74\,nm}$

b. $E_2 = 4E_1 = 4(8\times10^{-21}\,J) = 3.2\times10^{-20}\,J$

since $V=0$, $E_2 = \frac{p^2}{2m} \implies p = \sqrt{2mE}$

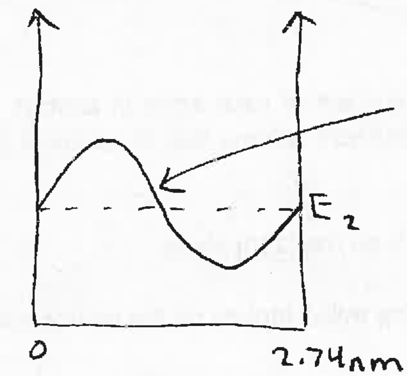
Note:
$E = hc/\lambda$
only applicable for photons

$$p = \sqrt{2(9.11\times10^{-31}\,kg)(3.2\times10^{-20}\,J)} = 2.415\times10^{-25}\ \frac{kg\,m}{s}$$

$$p = \hbar k = \frac{\hbar\,2\pi}{\lambda} \implies \lambda = \frac{\hbar\,2\pi}{p}$$

$$\lambda = \frac{(1.054\times10^{-34}\ J\cdot s)\,2\pi}{2.413\times10^{-25}\ \frac{kg\,m}{s}} = 2.74\times10^{-9}\ m \ \boxed{= 2.74\,nm}$$

* We could also solve this by recognizing that the E_2 state looks like this



one wavelength is the width of the well

* Similarly, the wavelength of an electron in E_4 level would be $\frac{2.74nm}{2}$.

In E_1, $\lambda = 2\cdot 2.74nm = 5.48nm$

c. For probability, we need $\int \psi\cdot\psi^*\,dx$, $E_1 \Rightarrow n=1$

$$\int_0^{a/4} \frac{2}{a}\sin^2\left(\frac{\pi}{a}x\right)dx = \frac{2}{a}\int_0^{a/4}\left[\frac{1}{2} - \frac{1}{2}\cos\left(\frac{2\pi}{a}x\right)\right]dx$$

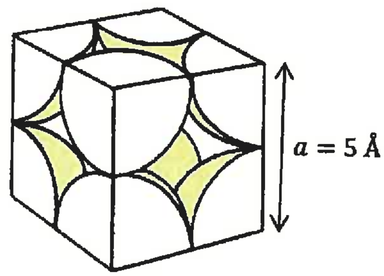
$$= \frac{2}{a}\left[\frac{1}{2}x\Big|_0^{a/4} - \frac{1}{2}\,\frac{\sin\left(\frac{2\pi}{a}x\right)}{2\pi/a}\Bigg|_0^{a/4}\right] = \frac{2}{a}\left[\frac{a}{8} - \left[\frac{1}{2}\cdot\frac{a}{2\pi}\right]\right]$$

$$= \frac{1}{4} - \frac{1}{2\pi}\ \boxed{= 0.091}$$

d. See plot $E_1 = 50meV$, $E_2 = 200meV$, $E_3 = 450meV$

(25 points)

2. Consider a simple cubic (SC) lattice unit cell with lattice constant $a = 5$ Å as shown below



(a) Assuming each atom is a hard sphere with the surface of each atom in contact with its nearest neighbor, calculate the percentage of total unit cell volume that is occupied (packing fraction). Show your work!

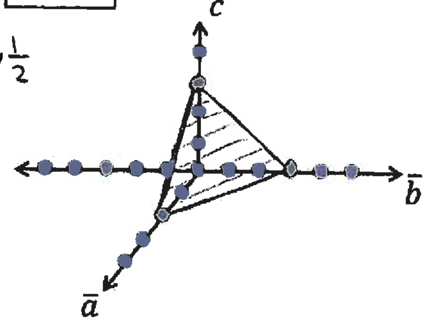
(b) Calculate the surface atomic density (in atoms/cm^2) on the (110) plane.

(5 points) (c) Sketch the three planes represented by the following miller indices on the empty axes:

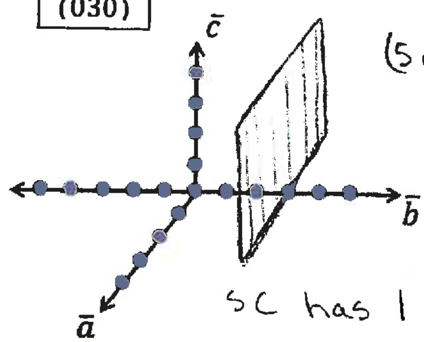
(322)

$(322) \rightarrow \frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

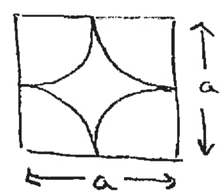
$\rightarrow 2, 3, 3$



(030)



(a)
(5 points)



$a = 2r$

$V_{sphere} = \frac{4}{3}\pi\left(\frac{a}{2}\right)^3 = \frac{\pi}{6}a^3$

SC has 1 atom per unit cell

so $V_{sphere\ total} = \frac{\pi}{6}a^3$

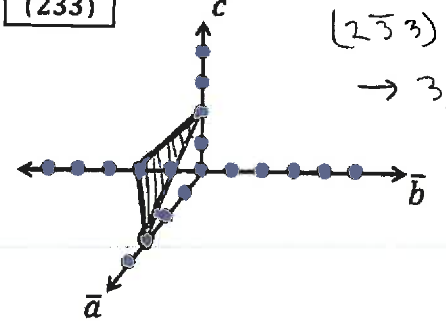
$PF = \frac{V_{sphere\ total}}{V_{unit\ cell}} = \frac{\frac{\pi}{6}a^3}{a^3} = \frac{\pi}{6}$

$\boxed{= 0.524 \text{ or } 52.4\%}$

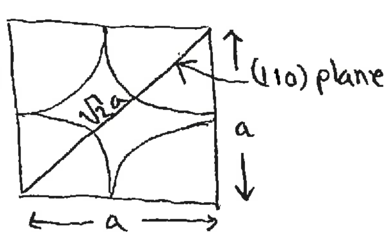
$(2\bar{3}3)$

$(2\bar{3}3) \rightarrow \frac{1}{2}, -\frac{1}{3}, \frac{1}{3}$

$\rightarrow 3, -2, 2$



(b)
5 points)
top view



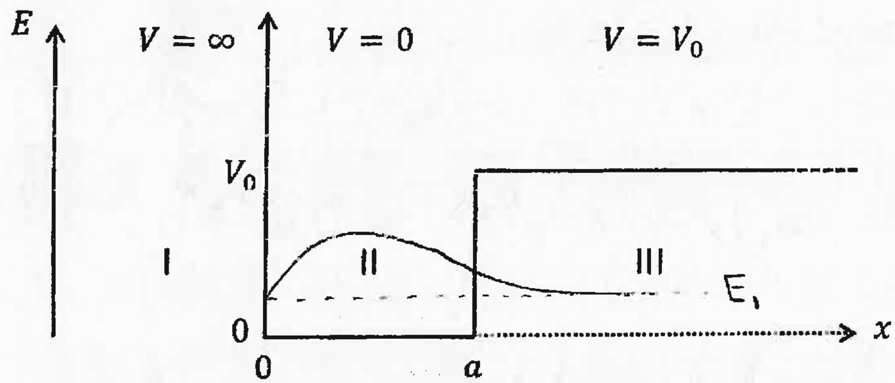
area of plane is $a \cdot \sqrt{2}a = \sqrt{2}a^2$

plane intercepts $\frac{1}{4} \times 4 = 1$ atom

$SD_{(110)} = \frac{1 \text{ atom}}{\sqrt{2}(5 \times 10^{-8} cm)^2} = \boxed{2.83 \times 10^{14} \frac{atoms}{cm^2}}$

(25 points)

3. A particle with mass m and fixed total energy E, where $0 < E < V_0$, is placed in the one-dimensional potential well shown below. You can assume there are no additional interfaces to the right of $x = a$.



a. (5 points) Write expressions for the time-independent Schrodinger equation and the wave numbers (k_2 and k_3) in regions II and III. k should be real in both regions.

b. (5 points) Write down the general solutions to the time-independent Schrodinger equation in regions II and III.

c. (5 points) Write down the four boundary conditions and simplify your general solutions from part (b) so they make physical sense.

d. (5 points) Using the boundary conditions, find two simultaneous equations relating k_2 and k_3.

e. (5 points) By manipulating the equations from part (d), show that the equation we would need to solve to determine the particle energies is

$$\tan(k_2 a) = -\frac{k_2}{k_3} = -\sqrt{\frac{E}{V_0 - E}}$$

***Extra credit.* (3 points)** Sketch the approximate shape of the wave function for the first bound state on the potential profile above.

a. $\frac{d^2\psi_2}{dx^2} + \frac{2mE}{\hbar^2}\psi_2 = 0$ $\quad k_2 = \sqrt{\frac{2mE}{\hbar^2}}$ region II

$\frac{d^2\psi_3}{dx^2} - \frac{2m(V_0-E)}{\hbar^2}\psi_3 = 0$ $\quad k_3 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ region III

* k_3 real

so we have

region II: $\frac{d^2\psi_2}{dx^2} + k_2^2\psi_2 = 0$

region III: $\frac{d^2\psi_3}{dx^2} - k_3^2\psi_3 = 0$

b. Solutions to T.I.S.E.

$$\left.\begin{aligned} &\text{region II:} \quad \psi_2(x) = A\sin(k_2x) + B\cos(k_2x) \\ &\text{region III:} \quad \psi_3(x) = Ce^{k_3x} + De^{-k_3x} \end{aligned}\right\} \text{general solutions}$$

c. Four boundary conditions

1. $\psi_2(0) = 0$ Using (1), we know $B = 0$
2. $\psi_3(\infty) = 0$ so $\psi_2(x) = A\sin(k_2x)$
3. $\psi_2(a) = \psi_3(a)$ Using (2), we know $C = 0$
4. $\psi_2'(a) = \psi_3'(a)$ so $\psi_3(x) = De^{-k_3x}$

d. Using (3) $\Longrightarrow$ $A\sin(k_2a) = De^{-k_3a}$

Using (4) $\Longrightarrow$ $Ak_2\cos(k_2a) = -Dk_3e^{-k_3a}$

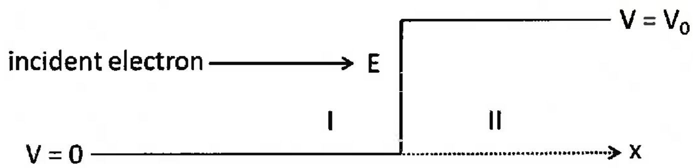
e. Divide equations in d

$$\frac{A\sin(k_2a)}{Ak_2\cos(k_2a)} = \frac{De^{-k_3a}}{-Dk_3e^{-k_3a}} \Longrightarrow \tan(k_2a) = -\frac{k_2}{k_3} = -\sqrt{\frac{E}{V_0-E}}$$

Extra Credit: See plot

5 Multiple Choice Questions: (6 points each)

1. Consider an electron incident on the step potential barrier with $E<V_0$ as shown below. What is the nature of the wave function in region I?



(a) Decaying exponential
(b) Travelling wave in the positive x direction
(c) Traveling wave in the negative x direction
(d) Travelling wave in the positive *and* negative x directions

2. An electron's uncertainty in position is no greater than 2 Å. Determine the minimum uncertainty in momentum (in kg-m/s).

(a) 1.7e-25
(b) 8.4e-26
(c) 8.4e-26
(d) 5.3e-25

3. What is the ordering of the number of atoms per unit cell ordered from highest (left) to lowest (right)
(a) SC, BCC, FCC
(b) FCC, BCC, SC
(c) BCC, FCC, SC
(d) FCC, SC, BCC

4. Which lattice structure has the highest packing fraction (volume of the unit cell that is occupied)?
(a) FCC
(b) BCC
(c) SC
(d) Diamond

5. Fill in the blanks: Silicon forms in the diamond lattice structure. GaAs forms in the zinc blende lattice structure.

Some Relevant Equations and Constants:

$\hbar = h/(2\pi) =$ 1.054 x 10^{-34} J s

$m_0 =$ 9.11 x 10^{-31} kg

q = 1.6 x 10^{-19} C

c = 3 x 10^{8} m/s

$$\sin^2 x = \frac{1}{2} - \frac{\cos 2x}{2}$$

(Time-independent Schrodinger equation): $\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi(x) = 0$